201-16037B

I U C L I D

Data Set

Existing Chemical	:	ID: 15890-25-2
CAS No.	:	15890-25-2
EINECS Name	:	tris(dipentyldithiocarbamato-S,S')antimony
EC No.	:	240-028-2
Molecular Formula	:	C33H66N3S6Sb

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	21.01.2004

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	21.01.2004
Status	:	
Memo	:	RT Vanderbilt
Printing date	:	29.01.2004
Revision date	:	
Date of last update	:	29.01.2004
Number of pages	:	18
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 345 - °C
Sublimation	:	
Method	:	other: estimated with Epiwin
Year	:	2004
GLP	:	no
Test substance	:	
Result	:	Melting Pt (deg C): 345.05 (Mean or Weighted MP)
Source	:	Epona Associates, LLC
Test condition	:	MPBPWIN v1.41
Test substance	:	SMILES : [Sb](SC(=S)N(CCCCC)CCCCC)(SC(=S)N(CCCCC)CCCCC)SC(=S)N(CCCCC)CCCCC CHEM : Antimony, tris(dipentylcarbamodithioato-S,S)-, (oc-6-11)- CAS NUM: 015890-25-2 MOL FOR: C33 H66 N3 S6 Sb1 MOL WT : 819.03
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.01.2004 (2)

2.2 BOILING POINT

Value	:	= 784 - °C at 1013 hPa
Decomposition	:	
Method	:	other: estimated using Epiwin
Year	:	2004
GLP	:	no
Test substance	:	
Result	:	Boiling Pt (deg C): 783.55 (Adapted Stein & Brown method)
Source	:	Epona Associates, LLC
Test condition	:	MPBPWIN v1.41
Test substance	:	SMILES : [Sb](SC(=S)N(CCCCC)CCCCC)(SC(=S)N(CCCCC)CCCCC)SC(=S)N(CCCCC)CCCCC CHEM : Antimony, tris(dipentylcarbamodithioato-S,S)-, (oc-6-11)- CAS NUM: 015890-25-2 MOL FOR: C33 H66 N3 S6 Sb1 MOL WT : 819.03
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.01.2004 (2)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	< 0 - hPa at 25 °C

Decomposition	:	
Method	:	other (calculated)
Year	:	2004
GLP	:	no
Test substance	:	
Result	:	VP (mm Hg,25 deg C): 2.07E-019 (Modified Grain method)
Source	:	Epona Associates, LLC
Test condition	:	MPBPWIN v1.41
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.01.2004 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= 12.7 - at 25 °C
pH value	:	-
Method	:	other (calculated)
Year	:	2004
GLP	:	no
Test substance	:	
Result	:	Log Kow (KOWWIN v1.67 estimate) = 12.69
Source	:	Epona Associates, LLC
Test condition	:	KOWWIN v1.67 estimate
Test substance	:	SMILES : [Sb](SC(=S)N(CCCCC)CCCCC)(SC(=S)N(CCCCC)CCCCC)SC(=S)N(CCCCC)CCCCC CHEM : Antimony, tris(dipentylcarbamodithioato-S,S)-, (oc-6-11)- CAS NUM: 015890-25-2 MOL FOR: C33 H66 N3 S6 Sb1 MOL WT : 819.03
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.01.2004 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	- at °C
pH value	:	-
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	other: estimated using Epiwin
Year	:	2004
GLP	:	no
Test substance	:	
Result	:	Water Sol Estimate from Fragments: Wat Sol (v1.01 est) = 0.0008742 mg/L Water Solubility at 25 deg C (mg/L): 8.289e-010

Source	:	Epona Associates, LLC
Test condition	:	Water Solubility Estimate from Log Kow (WSKOW v1.41): log Kow used: 12.69 (estimated); no-melting pt equation used
Test substance	:	SMILES : [Sb](SC(=S)N(CCCCC)CCCCC)(SC(=S)N(CCCCC)CCCCC)SC(=S)N(CCCCC)CCCCC CHEM : Antimony, tris(dipentylcarbamodithioato-S,S)-, (oc-6-11)- CAS NUM: 015890-25-2 MOL FOR: C33 H66 N3 S6 Sb1 MOL WT : 819.03
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

22.01.2004 (1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

DIRECT PHOTOLYSIS		
Halflife t1/2	:	= 26 - minute(s)
Degradation	:	- % after
Quantum yield	:	
INDIRECT PHOTOLYSIS		
Sensitizer	:	
Conc. of sensitizer	:	
Rate constant	:	ca. .000000000286 cm^3/(molecule*sec)
Degradation	:	- % after
Deg. product	:	
Method	:	other (calculated)
Year	:	2004
GLP	:	no
Test substance	:	
Result	:	Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 286.9573 E-12 cm3/molecule-sec Half-Life = 0.037 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 26.837 Min Ozone Reaction: No Ozone Reaction Estimation
Source	:	Epona Associates, LLC
Test condition	:	Atmospheric Oxidation (25 deg C) [AopWin v1.91]
Test substance	:	SMILES : [Sb](SC(=S)N(CCCCC)CCCCC)(SC(=S)N(CCCCC)CCCCC)SC(=S)N(CCCCC)CCCCC CHEM : Antimony, tris(dipentylcarbamodithioato-S,S)-, (oc-6-11)- CAS NUM: 015890-25-2 MOL FOR: C33 H66 N3 S6 Sb1 MOL WT : 819.03
Reliability	:	(2) valid with restrictions

29.01.2004 (2)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)

Soil : % (Fugacity Model Level II/III)
Method : other: estimated using Epiwin
Year : 2004

Result : Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0652	0.894	1000
Water	7.24	360	1000
Soil	28.5	360	1000
Sediment	64.2	1.44e+003	0

Persistence Time: 627 hr

Source : Epona Associates, LLC
Test substance : SMILES :
[Sb](SC(=S)N(CCCCC)CCCCC)(SC(=S)N(CCCCC)CCCCC)SC(=S)N(CCCCC)CCCCC
CHEM : Antimony, tris(dipentylcarbamodithioato-S,S)-, (oc-6-11)-
CAS NUM: 015890-25-2
MOL FOR: C33 H66 N3 S6 Sb1
MOL WT : 819.03
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
22.01.2004 (2)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 16400 - mg/kg bw
Species	:	rat
Strain	:	other: albino
Sex	:	male/female
Number of animals	:	36
Vehicle	:	other: cottonseed oil
Doses	:	1.0, 2.1, 4.1, 8.2, 11.6, and 16.4 gm/kg
Method	:	
Year	:	1961
GLP	:	no
Test substance	:	
Result	:	At the higher levels of dosage the rats showed symptoms of depression and excessive laxation, and at the highest level also became prostrated. These symptoms subsided within 24 hours. The animals appeared normal throughout the remainder of the observation period. No deaths occurred, and the post-mortem examinations disclosed no gross pathology.
Source	:	Epona Associates, LLC
Test condition	:	Six groups of rats (3/sex/dose) were fasted for approximately 20 hours and orally dosed with the test material in the form of 10 to 40 per cent suspensions in cotonseed oil. Animals were observed for appearance, behavior, body weight and mortality for 14 days and then sacrificed and examined grossly.
Test substance	:	Antimony dialkyldithiocarbamate
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

29.01.2004 (4)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	= 16000 - mg/kg bw
Species	:	rabbit
Strain	:	other: albino
Sex	:	male/female
Number of animals	:	12
Vehicle	:	water
Doses	:	0.25, 1, 4, 8 and 16 gm/kg
Method	:	
Year	:	1960
GLP	:	no data
Test substance	:	
Result	:	There was no mortality and all animals gain in body weight and appeared to be in good health during the observation period. Slight localized erythema was observed at the end of the 24-hour exposure period at all dose levels. This receded after the fourth day and the skin was normal at 7

days. Post-mortem examinations disclosed no gross pathology.

Source	:	Epona Associates, LLC
Test condition	:	Five groups of rabbits (2 males/dose at the 4 lower doses; 3 males and 1 female at the highest dose) were depilated over the entire trunk and an area of about 1 square inch was abraded. Doses of the test material in the form of 25 to 60 per cent aqueous pastes were applied to the skin and maintained for a 24-hour period under a plastic sleeve. After 24 hours, the excess material was washed off and the animals were observed for appearance, behavior, body weight, and mortality for 14 days. Skin irritation was scored according to Draize. The animals were sacrificed and examined grossly after the observation period.
Test substance	:	Antimony dialkyldithiocarbamate
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

29.01.2004 (3)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella strains TA98, TA100, TA1535, TA1537 and TA1538
Test concentration	:	100, 333, 1000, 3333, 5000 ug/plate
Cycotoxic concentr.	:	> 5000 ug/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: Ames et al (1975)
Year	:	1992
GLP	:	yes
Test substance	:	
Result	:	The results of the dose range finding study indicate that a slight precipitate of the test substance forms, but no appreciable toxicity was observed. In the mutagenicity assay no positive responses were observed with any of the tester strains in the presence or absence of metabolic activation. Precipitate, but no appreciable toxicity was observed.
Source	:	Epona Associates, LLC
Test condition	:	The assay was performed in two phases using the plate incorporation method, in the presence and absence of metabolic activation. The first phase, the dose range finding study, was used to establish the dose range for the mutagenicity assay. In the dose range finding study, the maximum dose tested was 5000 ug/plate. The test substance was dissolved in acetone. The second phase, the mutagenicity assay, was used to evaluate the mutagenicity of the test substance. In the mutagenicity assay, the dose

levels were 100, 333, 1000, 3333, 1000 and 5000 ug/plate.

Test substance : Antimony dipentyldithiocarbamate; lot EVR-384-281
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
29.01.2004 (6)

5.6 GENETIC TOXICITY 'IN VIVO'

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : ICR
Route of admin. : i.p.
Exposure period :
Doses : 1250, 2500 or 5000 mg/kg
Result :
Method : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year : 1992
GLP : yes
Test substance :

Result : In the absence of mortality in the pilot study, the maximum dose level used for the micronucleus study was 5000 mg/kg. No mortality or clinical signs were observed in the micronucleus assay. Bone marrow cells, collected at 24, 48, or 72 hours after treatment, did not show a reduction in the ratio of polychromatic erythrocytes to total erythrocytes suggesting the test substance did not induce bone marrow toxicity. No significant increase in micronucleated polychromatic erythrocytes was observed at 24, 48 or 72 hours after dose administration in the male mice. A significant increase in micronucleated polychromatic erythocytes was observed at dose levels of 2500 and 5000 mg/kg in female mice, only at the 48 hour sampling time.

In the confirmatory assay, no mortality or clinical signs were observed in either male or female animals. No reduction in the ratio of polychromatic erythrocytes to total erythrocytes was observed in any treatment group, suggesting the test substance did not induce bone marrow toxicity. No significant increase in micronucleated polychromatic erythrocytes was observed in the male mice; a significant increase in micronucleated polychromatic erythrocytes was observed at dose levels of 2500 and 5000 mg/kg in female animals.

Source : Epona Associates, LLC
Test condition : Male and female ICR mice were exposed to 1250, 2500 or 5000 mg/kg of the test substance which was administered in a total volume of 20 ml/kg as a single ip injection. The vehicle used was corn oil. For the micronucleus assay, animals were assigned to 13 groups of 5 animals/sex. An additional group of 5 animals/sex was designated as replacement animals and were dosed with the high dose of test substance in case of mortality prior to scheduled sacrifice. 5 animals/sex/group were sacrificed after 24, 48 and 72 hours following dose administration. 5 animals/sex were administered a positive control (cyclophosphamide, 30 mg/kg) and sacrificed after 24 hours.

Polychromatic erythrocytes were scored for the presence of micronuclei. The number of micronucleated normocytes in the field of 1000 polychromatic erythrocytes was enumerated. The proportion of polychromatic erythrocytes to total erythocytes counted was also recorded.

In the confirmatory micronucleus assay 6 animals per sex were assigned to four groups (vehicle control, 2500 and 5000 mg/kg, and positive control) and sacrificed after 48 hours. Bone marow cells were collected at

examined for micronucleated polychromatic erythrocytes.

Test substance : Antimony dipentyldithiocarbamate; lot EVR-384-281

Conclusion : The results of the initial and confirmatory assay indicate that under the conditions of this study, the test substance did induce a significant increase in micronucleated polychromatic erythrocytes in female ICR mice. Significant inter-animalvariability was observed in the dose groups that were signiifacntly elevated above the vehicle control group. The test substance was concluded to be weakly positive in the mouse micronucleus assay.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

29.01.2004 (5)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Water Solubility Estimate from Log Kow (WSKOW v1.41)

(2) EPIWIN v. 3.11

(3) Food and Drug Research Laboratories, Inc. (1961) The Acute Dermal Toxicity for Rats of Antimony Diamyl Dithiocarbamate (Compound OD 596). Laboratory No. 81447

(4) Food and Drug Research Laboratories, Inc. (1961) The Acute Oral Toxicity for Rats of Compound OD 596. Laboratory No. 81447A

(5) Putnam, DI and Morris, MJ (1992) Micronucleus Cytogenetic Assay in Mice, Antimony Dipentyldithiocarbamate. Microbiological Associates, Inc. Study Number TA214.122

(6) San, RHC and Sly, JE (1992) Salmonella/Mammalian-Microsome Plate Incorporation Mutagenicity Assay (Ames Test), Antimony Dipentyldithiocarbamate. Microbiological Assocaites, Inc. Study Number TA214.501.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT